Jusong Yu

Computational Physicist, Ph.D.

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Expertise Synopsis (Software Engineering)

Backend Core developer of AiiDA (open-source workflow system for computational science). Designed high-performance asynchronous task runtime in **Python**. Leading core redesign using **Rust** for scalability and multi-threading support, including the design of a new domain-specific language (with the interpreter implement in Rust) for intuitive workflow creation.

Frontend Coordinated AiiDA lab development (web-based graphical frontend for AiiDA). Built interactive web applications using Javascript, htmx, plot.ly dash and Jupyter notebooks.

DevOps Experienced with **Docker** and **kubernetes**. Deployed AiiDA lab servers and integrated containerization capabilities into AiiDA.

Numerical Solver Developed an atomic Schrödinger equation solver in **Julia** for optimizing the pseudopotential approximation in materials simulations.

High-performance computing User of tier-0 supercomputers; background in **C/C++**

Expertise Synopsis (Scientific)

Predicting electronic properties of novel materials through quantum mechanical simulations, solving materials challenges together with experimentalists. Co-authored $>$ 20 peer-reviewed papers, $>$ 700 citations, h-index of 14 (*Google Scholar*).

Professional experience

2022-today **Paul Scherrer Institut (PSI)**, *Switzerland*, Postdoctoral scientist, LMS lab

- **Redesign the core architecture of the AiiDA workflow manager** migrating performance-critical components to **Rust** to unlock the power of multithreading and replace a small-file storage tool with 10x faster **Rust** implementation. Also created a domain-specific language for writing workflows that can be embedded in Python scripts.
- **Coordinated the development of AiiDA lab**(aiidalab.net), the web-based graphical frontend for AiiDA, and delivered its first stable release to stakeholders. Drove standardization around vscode container-based development workflows and enforce coding standard, boosting the team's monthly contributions. Authored Kubernetes deployment templates and deployed an institute internal production instance that now serves $>$ 10 active experimental researchers.
- **Developed PseudopotentialGenerator.jl**, an atomic Schrödinger solver in **Julia** that integrates with the language's optimization libraries to generate high-quality pseudopotentials for density-functional-theory simulations.
- **Migrated the AiiDA user community** from Google Groups to a Discourse forum, reviving discussions and increasing active participation.
- **Successfully supervised a Google Summer of Code 2022 student** that built a ranking system for the AiiDA plugin registry, turning it into one of the community's most-visited sites.
- Co-authored 3 peer-reviewed research papers, include one published in Nature Reviews Physics

2021-2022 **EPF Lausanne**, *Switzerland*, Postdoctoral scientist, THEOS groups

- **Co-lead of a work package of the EU Horizon 2020 MARKETPLACE project**, contributing to the consortium and leading the development of HPC-resource integration as a service.
- **Lead maintainer of ipyoptimade**, a Jupyter-widget and Voilà application for OPTIMADE (Open Databases Integration for Materials Design); delivered critical core fixes that have kept the web app production-stable for over 15 months.
- Adapted the AiiDA workflow manager (aiida.net) to automate approximation verification in materials simulations.

2017-2021 **South China University of Thechnology**, *China*, Ph.D student
Topic: Discovery of novel two-dimensional materials using cluster-expansion and machine-learning methods.

- **Authored the group's flagship crystal structure generation tool**, adopted across the team and showcased in a dedicated workshop.
- Build and maintain a high-performance computing (HPC) cluster for the research group.
- Primary author of Libxc.jl, a Julia interface to the *libxc* exchange–correlation functional library, now widely used in Julia-based DFT simulations.
- Co-authored 4 peer-reviewed research papers.

2014-2017 **Chinese Academy of Science**, *China*, M.Sc.
Topic: Method development and simulation for material nonlinear optical properties and excited-state phenomena.

- Co-authored 7 peer-reviewed research papers, in close collaboration with experimentalist at Laboratory.

Education

2017-2021 **Ph.D in Physics**, *South China University of Thechnology*
Course in basic quantum computing, computational physics, scientific programming in Julia, various computational materials codes (QE, VASP, LAMMPS ...), developing skills in teaching

2014-2017 **M.Sc. Physics**, *Chinese Academy of Science*, China, GPA 5/6
Courses in mathematical method for physicists, solid state physics, computational quantum physics, scientific programming in python, scientific writing & editing

2010-2014 **B.Sc. Polymer science**, *Northwestern Polytechnical University*, China, GPA 5/6
Courses in analysis, linear algebra, organic chemistry, C/C++, quantum mechanics

Awards

2012-2013 **University Scholarship to support exchange studies in Taiwan**, *(~1.5k EUR)*

2011-2012 **University Department Scholarship (for top 5% student)**, *(~1k EUR)*

Invited talks

2024.10 **MolSSI Workshop on Julia for Computational Molecular and Materials Science**, *MolSSI*, Pittsburgh, PA, USA
AiiDA: a DSL, an ecosystem

2024.03 **American Physical Society Conference**, *APS*, Minneapolis, MN, USA
Reproducible workflows for verification and optimization of solid-state pseudopotentials

2023.10 **Huawei Thames Summit & European Innovation Star Workshop**, *Huawei*, Cambridge, United Kingdom
Accelerating materials-science research via reproducible simulations with AiiDA and Materials Cloud

2022.06 **OPTIMADE Workshop at CECAM**, *EPFL*, Lausanne, Switzerland
Integrating Materials Cloud databases with OPTIMADE

Further Activities

2024-today **Host and Organizer, Weekly Rust Learning Sessions**, *Paul Scherrer Institut*
Organize and lead weekly sessions to teach Rust programming, helping colleagues adopt Rust for daily work.

2022-today **Project contact person, *NumFOCUS* affiliated project**
NumFOCUS is a non-profit organization that promotes open practices in research, data, and scientific computing. It serves as the fiscal sponsor of many key open-source scientific software projects, including NumPy, SciPy, Julia.

2016-today **Reviewer for scientific journals**, *PCCP, CMS, JPCA*

Personal Information

Nationality	Chinese
Current Residence	Switzerland
Resident Permit	Permit B
Languages	English, Chinese, German(A2)

References

Dr. Giovanni Pizzi, *Materials Software and Data Group*, Paul Scherrer Institut (PSI)
Phone +41 56 310 58 24, giovanni.pizzi@psi.ch, profile page
Giovanni is the group leader of Materials Software and Data Group at PSI and coordinates the AiiDA/AiiDA lab and scientific project. He is the person I have worked with most closely at EPFL and PSI.

Prof. Nicola Marzari, *Institute of Materials Science and Engineering*, EPFL
Phone +41 21 693 1129, nicola.marzari@epfl.ch, profile page
Nicola leads the THEOS group at EPFL. He is also the director of the Swiss MARVEL project, and former chairman of the European Psi-k network. I have worked closely with Nicola on scientific project and on numerous desigin decision on AiiDA lab.